

Emergence of thermodynamic behavior within composite quantum systems

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Abstract

Entanglement within a given device provides a potential resource for quantum information processing. Entanglement between system and environment leads to decoherence (thus suppressing non-classical features within the system) but also opens up a route to robust and universal control. The latter is related to thermodynamic equilibrium, a generic behavior of bi-partite quantum systems. Fingerprints of this equilibrium behavior (including relaxation and stability) show up already far from the thermodynamic limit, where a complete solution of the underlying Schrödinger dynamics of the total system is still feasible.

Key words: Decoherence, Quantum statistical mechanics, Nonequilibrium and irreversible thermodynamics

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1. Introduction

There have been various attempts to reduce thermodynamics to some underlying more fundamental theory. While the vast majority of the pertinent work done in this field has been based on classical mechanics [1], a reduction to quantum mechanics has also attracted increasing interest [2]. Decoherence [3] has, during the last years, often been discussed as one of the main obstacles for the implementation of large-scale quantum computation. Quantum thermodynamics [4], on the other hand, tries to show that decoherence is far from being just a technical nuisance but a generic phenomenon of partite quantum systems giving rise to

some of the most dominating, if classical, features of closed (finite) quantum systems: thermal equilibrium.

The program of a quantum foundation of thermodynamics should contain the following points:

(1) a definition of thermodynamic quantities (in the ideal case, as a function of microstates); (2) a derivation of the second law of thermodynamics under appropriate constraints (including stability, irreversibility, universality); (3) a justification of the Gibbsian fundamental form (state functions and conjugate variables); (4) a proof of extensivity or intensivity, respectively, of the thermodynamic variables; (5) a characterization of thermodynamic systems (as opposed to other systems); (6) a kind of correspondence principle (explaining the efficiency of standard classical approaches despite their underlying quantum nature).

Here we cannot do justice to this rather challenging program. Instead we want to address some of the main results available to us.

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2. The Model

We consider a bipartite system – an observed system or gas g and an environment or container c , described by the Hamiltonian

$$\hat{H} = \hat{H}^g + \hat{H}^c + \hat{I} . \quad (1)$$

Note that also the environment requires a full quantum treatment and should not be replaced by (classical) boundary conditions. \hat{I} defines the interaction between these two subsystems.

Weak coupling between system and environment has routinely to be assumed in standard thermodynamics [5]; otherwise the concept of intensive and extensive variables would lose its meaning. Furthermore, in this case the full spectrum of the coupled system will not look significantly different from the one that results from a mere convolution of the two spectra of the uncoupled system. To quantify the weak coupling precondition, we require

$$\sqrt{\langle \hat{I}^2 \rangle} \ll \langle \hat{H}^g \rangle, \langle \hat{H}^c \rangle . \quad (2)$$

This inequality must hold for all states that the total system can possibly evolve into under given constraints.

The weak coupling has further to be classified. Not so much for practical, but for theoretical reasons, the most important contact conditions are the *microcanonical* and the *canonical* conditions. In the microcanonical contact scenario no energy transfer between system and environment is allowed, as opposed to the canonical contact.

3. Microcanonical Conditions

If a system is thermally isolated, it is not necessarily isolated in the microscopic sense, i.e., not uncoupled to any other system. The only constraint is that the interaction with the environment should not give rise to any energy exchange. As will be seen later, this does not mean that such an interaction has no effect on the considered system, a fact that might seem counterintuitive from a classical point of view. This constraint, however, leads to an immense reduction of the region in Hilbert space which the wave vector is allowed to enter. This reduced area is called “accessible region” of the system.

3.1. Accessible Region (AR)

If the energies contained in the gas g and the environment c , respectively,

$$E^g := \langle \hat{H}^g \rangle , \quad E^c := \langle \hat{H}^c \rangle \quad (3)$$

are to be conserved, i.e. if these two energies are constants of motion, the following commutator relations should hold

$$[\hat{H}^g, \hat{H}] = 0 , \quad [\hat{H}^c, \hat{H}] = 0 . \quad (4)$$

It then follows from

$$[\hat{H}^g, \hat{H}] = [\hat{H}^g, \hat{H}^g] + [\hat{H}^g, \hat{H}^c] + [\hat{H}^g, \hat{I}] = 0 \quad (5)$$

that

$$[\hat{H}^g, \hat{I}] = 0 , \quad [\hat{H}^c, \hat{I}] = 0 . \quad (6)$$

Except for these constraints we need not specify \hat{I} in more detail. All interactions that fulfill this relation will create perfectly microcanonical situations, regardless of their strength or any other feature. And, as will be shown, there are a lot of possible interactions that do fulfill these conditions and create entanglement and therefore give rise to the increase of local entropy.

Due to (4) the local energy projectors \hat{P}_A^g of the gas system and \hat{P}_B^c of the container

$$\hat{P}_A^g = \sum_a |A, a\rangle \langle A, a| , \quad \hat{P}_B^c = \sum_b |B, b\rangle \langle B, b| \quad (7)$$

commute with the full Hamiltonian,

$$[\hat{P}_A^g, \hat{H}] = [\hat{P}_B^c, \hat{H}] = 0 . \quad (8)$$

Here $a(b)$ specify the degenerate states (degeneracies $N_A(N_B)$) for given energy eigenvalue $A(B)$ in the gas (container) system. Thus, because the system is not allowed to exchange energy with the environment the joint probability W_{AB} must be conserved

$$\begin{aligned} \langle \psi | \hat{P}_A^g \hat{P}_B^c | \psi \rangle &= \sum_{a,b} \left| \psi_{ab}^{AB}(t) \right|^2 = \sum_{a,b} \left| \psi_{ab}^{AB}(0) \right|^2 \\ &= W_{AB} , \end{aligned} \quad (9)$$

and is set by the initial state. This means that the energy probability distribution $\{W_{AB}\}$ is a constant of motion. Vice versa, any state that features this same energy probability distribution as the initial state belongs to the accessible region and could possibly be reached during microcanonical dynamics.

In the following we mainly consider initial product states, states that have zero local entropy in the beginning and for which

$$\sum_{a,b} \left| \psi_{ab}^{AB}(0) \right|^2 = \sum_{a,b} \left| \psi_a^A(0) \right|^2 \left| \psi_b^B(0) \right|^2 = W_A W_B. \quad (10)$$

This is the only constraint that microcanonical conditions impose on the accessible region of Hilbert space. Note that this does not mean that local entropy is constant.

3.2. The “Landscape” of P^g in the Accessible Region

To demonstrate that the largest part of the accessible region is filled with states of almost minimum purity (maximum entropy), we proceed as follows:

- (i) First we compute the (unique) state with the lowest possible purity, $\hat{\rho}_{\min}^g$ (with purity $P(\hat{\rho}_{\min}^g) = P_{\min}^g$) that is consistent with the given initial state and the microcanonical conditions, consequently with a given energy probability distribution $\{W_A\}$.
- (ii) Then we compute the average of P^g over the total accessible Hilbert space region, denoted by $\llbracket P^g \rrbracket$.
- (iii) We show that this average purity is very close to the purity of the lowest possible purity state $\hat{\rho}_{\min}^g$ for a large class of systems. Considering only these systems, which then define the class of thermodynamic systems, we can conclude that $P^g \approx P_{\min}^g$ for almost all states within the accessible region. Note that this conclusion is only possible because of the fact that the purity of $\hat{\rho}_{\min}^g$ is the absolute minimal purity which can be reached at all in the system. A quantity with a mean value close to a boundary cannot vary very much. Thus it is not possible that the distribution of the purity within the accessible region is something else but a very flat “lowland”, with a “soft depression” at $\hat{\rho}_{\min}^g$ (see Fig. 1) and a “peak” with $P^g = 1$.
- (iv) Since all states from the accessible region have the same energy probability distribution $\{W_A\}$ (remember (10)) and the minimum purity state $\hat{\rho}_{\min}^g$ is consistent with this distribution, all other states within the accessible region that feature $P^g \approx P_{\min}^g$ must yield reduced local

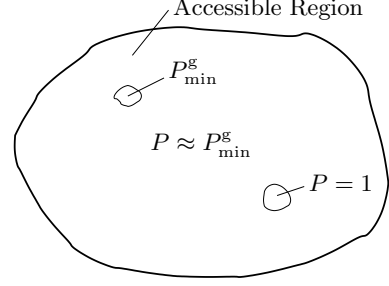


Fig. 1. Qualitative picture of the purity landscape in the microcanonical case. The biggest part of the accessible region is at $P \approx P_{\min}^g$ or at $P = P_{\min}^g$. There is however only a small zone featuring P significantly above P_{\min}^g or at the extreme $P = 1$. The only topological property this rough picture refers to is the relative size of different regions.

states that are very close to $\hat{\rho}_{\min}^g$ (in this context close means in terms of the distance measure $\text{Tr} \{(\hat{\rho}^g - \hat{\rho}_{\min}^g)^2\}$). Thus, as long as the trajectory keeps wandering through the compartment filled with those states the gas system is locally in a stationary state, equilibrium is reached.

Details can be found in Ref. [4,6].

3.3. Microcanonical Equilibrium

The minimal purity for subsystem g under the given constraints is

$$P_{\min}^g = \sum_A \frac{(W_A)^2}{N_A}. \quad (11)$$

For the Hilbert space average of P^g in the accessible region we find

$$\begin{aligned} \llbracket P^g \rrbracket &= \sum_A \frac{W_A^2}{N_A} \left(1 - \sum_B W_B^2 \right) \\ &+ \sum_B \frac{W_B^2}{N_B} \left(1 - \sum_A W_A^2 \right) \\ &+ \sum_{A,B} \frac{W_A^2 W_B^2 (N_A + N_B)}{N_A N_B + 1}. \end{aligned} \quad (12)$$

This average is thus a unique function of the invariants W_A, W_B , specified by the initial product state and the degeneracies N_A, N_B .

If the degeneracy of the occupied energy levels is large enough so that

$$N_A N_B + 1 \approx N_A N_B, \quad (13)$$

which should hold true for typical thermodynamic systems, (12) reduces to

$$\llbracket P^g \rrbracket \approx \sum_A \frac{(W_A)^2}{N_A} + \sum_B \frac{(W_B)^2}{N_B}. \quad (14)$$

The first sum in this expression is obviously exactly P_{\min}^g , so that for systems and initial conditions, in which the second sum is very small, the allowed region almost entirely consists of states for which $P^g \approx P_{\min}^g$. The second sum will be small if the container system occupies highly degenerate states typical for thermodynamic systems, in which the surrounding is much larger than the considered system. This is the set of cases mentioned already in Sect. 3.2: all systems fulfilling this pre-condition are called now *thermodynamic systems*. Thus we can conclude that all states within the accessible region are very close to $\hat{\rho}_{\min}^g$ and have approximately the purity P_{\min}^g . The density operator, which has $P^g = P_{\min}^g$ and $S^g = S_{\max}^g$, and which is consistent with the microcanonical conditions, is unique. The density operators with $P^g \approx P_{\min}^g$ should not deviate much from this one and should therefore also have $S^g \approx S_{\max}^g$, the latter being

$$S_{\max}^g = -k_B \sum_A W_A \ln \frac{W_A}{N_A}. \quad (15)$$

4. Energy Exchange Conditions

4.1. The Accessible and the Dominant Region

Our approach to the “energy exchange conditions” will be based on similar techniques as before. The possibility of a partition is still assumed. But now there is no further constraint on the interaction \hat{I} , since energy is allowed to flow from one subsystem to the other. The only constraint for the accessible region therefore derives from the initial state of the full system, and the fact that the probability to find the total system at some energy E ,

$$W(E) := \sum_{A,B/E} W_{AB} = \sum_{A,B/E} \sum_{a,b} |\psi_{ab}^{AB}|^2, \quad (16)$$

should be conserved, where $A, B/E$ stands for: all A, B such that $E_A^g + E_B^c = E$. This constraint is nothing else but the overall energy conservation.

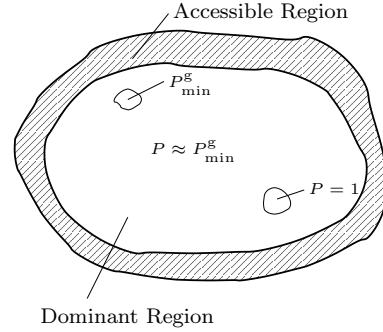


Fig. 2. Qualitative picture of the purity landscape. In the canonical case the accessible region contains a dominant region which almost entirely fills the accessible region. Within the dominant region, all states feature the same energy probability distribution. Thus all topology from the microcanonical case (cf. Fig. 1) transfers to the dominant region.

One could try to repeat the above calculation under the energy conservation constraint, but now it turns out that the average purity over the accessible region is no longer close to the actual minimum purity. Furthermore, the energy probability distribution of the individual considered system is no longer a constant of motion. Thus, we proceed in a slightly different way:

- (i) Contrary to the microcanonical case the probability to find the gas (container) subsystem at some given energy is no longer a constant of motion here. But one can prove that there is a predominant distribution, $\{W_{AB}^d\}$, which almost all states within the allowed region have in common. The subregion formed by these states is called the “dominant region”.
- (ii) Having identified the “dominant region” we demonstrate that this region is by far the biggest subregion in the accessible region of the system (see Fig. 2).
- (iii) Once the existence of such a dominant region has been established, we can use the results from the microcanonical conditions to argue that almost all states within this dominant region, which is specified by a fixed energy probability distribution for the considered system, feature the maximum local entropy that is consistent with the predominant distribution. Based on this analysis we get the equilibrium state of the considered system (see Sect. 4.2).

Just like in the previous case our subjective lack of

knowledge about where to find the system within the accessible region is irrelevant. The reduced local state $\hat{\rho}^g(t)$ as a function of the full state $|\psi(t)\rangle$ should always evolve into a state with a fixed probability distribution W_A , and an almost time invariant entropy, which is the maximum entropy consistent with this (canonical) distribution. Nevertheless, the state of the full system continues to move in Hilbert space with the constant velocity v ($v \approx$ energy uncertainty).

Again, details can be found in Ref. [4,6].

4.2. The Equilibrium State

Finally, to find the marginal, dominant energy probability distribution W_A^d of the gas system individually, one has to sum the compound probabilities W_{AB}^d over the irrelevant container system to obtain

$$\begin{aligned} W_A^d &= \sum_B W_{AB}^d = \sum_{B/E} \frac{N_A N_B}{\lambda_E} \\ &= N^g(E_A^g) \sum_{B/E} \frac{N^c(E_B^c) W(E)}{N(E)}, \end{aligned} \quad (17)$$

where again the sum over B/E denotes a summation under the condition $E = E_A^g + E_B^c$, and $N_A = N^g(E_A^g)$ and $N_B = N^c(E_B^c)$ are the respective degeneracies. Since $E_B^c = E - E_A^g$ is a function of E for fixed E_A^g we switch from a summation over B to a summation over E ,

$$W_A^d = N^g(E_A^g) \sum_E \frac{N^c(E - E_A^g) W(E)}{N(E)}. \quad (18)$$

This is the energy probability distribution for the gas system that one will find with overwhelming probability for a thermodynamic system. Simply by exchanging the indices (up to here everything is symmetric with respect to an exchange of the subsystems) we find the marginal dominant energy probability distribution for the container system.

So far we have only established the energy probability distributions for almost all states from the accessible region, but nothing has been said about entropy, purity, etc. The equilibrium state is still undetermined. Once the trajectory has entered the dominant region, we can assume that the trajectory will practically never leave it, because this region fills almost the whole accessible region of the system. But since all states within the dominant region feature the same energy probability distribution, motion within the dominant region

will never give rise to any further energy exchange between the subsystems. As a consequence the situation is as if the system was controlled by microcanonical conditions.

Therefore, we can take the arguments from Sect. 3.3 to identify the equilibrium state. Following this idea, we can start with (14) and use the dominant energy distribution W_{AB}^d , finding for the Hilbert space average of the purity of the gas

$$\llbracket P^g \rrbracket \approx \sum_A \frac{(W_A^d)^2}{N_A} + \sum_B \frac{(W_B^d)^2}{N_B}. \quad (19)$$

Once more it is possible to conclude that the second term (due to the environment) is much smaller than the first one for a sufficiently degenerate environment. The first term is exactly the minimum purity of the gas system within the dominant region. Thus, almost all states from the dominant region will yield approximately the same local gas state too. This equilibrium state $\hat{\rho}_{\text{eq}}^g$ is, again, the state of minimum purity (maximum entropy) that is consistent with the dominant energy distribution,

$$\hat{\rho}_{\text{eq}}^g \approx \sum_{A,a} \frac{W_A^d}{N_A} |A, a\rangle \langle A, a|. \quad (20)$$

One problem remains: the dominant energy probability distribution W_A^d (18) is not independent of the initial state since different energy probability distributions of the local initial state may result in different overall energy probability distributions $W(E)$, and those clearly enter (18) and thus even (20). Normally the canonical contact of standard thermodynamics leads to an equilibrium state, which does not depend on the initial state. The canonical contact turns out to be a special subclass, as we will demonstrate in the next Section.

5. Canonical Conditions

For a canonical situation the gas system should relax into the canonical equilibrium state, independent of the initial conditions. This behavior can be found, if a further condition is taken into account: a special form of the degeneracy of the environment N_B .

Let us assume an exponential increase of the container degeneracy

$$N_B = N_0^c e^{\alpha E_B^c}, \quad (21)$$

where α , N_0^c are some constants. Such a degeneracy structure is typical for modular systems [4]. We start again from (18) using (21) for the degeneracy of the environment

$$W_A^d = N_A e^{-\alpha E_A^g} \sum_E \frac{N_0^c e^{\alpha E} W(E)}{N(E)}. \quad (22)$$

Obviously, the sum does not depend on A at all. Since W_A^d has been constructed as some probability distribution it is still normalized by definition. Therefore the sum has to reduce to a normalizing factor. Finally we get for the dominant energy probability distribution of the gas system

$$W_A^d = \frac{N_A e^{-\alpha E_A^g}}{\sum_A N_A e^{-\alpha E_A^g}}. \quad (23)$$

This result is no longer dependent on the initial state!

The energy probability distributions of almost all states from the accessible region consistent with the constraints is then the canonical distribution: Since the argumentation for the minimal purity state (state of maximal entropy) remains unchanged, the equilibrium state reads now

$$\hat{\rho}_{\text{eq}}^g \approx \frac{1}{\sum_A N_A e^{-\alpha E_A^g}} \sum_{A,a} e^{-\alpha E_A^g} |A, a\rangle \langle A, a|. \quad (24)$$

Obviously, this is the well known canonical equilibrium state with the inverse temperature $\beta = \alpha$.

6. Temperature

One could claim that temperature should only be defined for equilibrium and thus there was no need to define it as a function of the micro state. Based on this reasoning temperature would then simply be defined as

$$\frac{1}{k_B T} = \frac{\partial S}{\partial E} = \frac{\partial}{\partial E} \ln G(E) = \frac{1}{G(E)} \frac{\partial G(E)}{\partial E}, \quad (25)$$

with $G(E)$ being the state density. In this way one would neglect all dynamical aspects (see [7]), since this definition is based on the Hamiltonian of the system rather than on its state. Strictly speaking, this definition would exclude all situations in which temperature appears as a function of time or space, because those are non-equilibrium situations.

A quantity like temperature is essentially determined by two properties: It should take on the same

value for two systems in energy exchanging contact, and if the energy of a system is changed without changing its volume, it should be a measure for the energy change per entropy change.

Most definitions rely on the second property. Maxwell connected the mean kinetic energy of a classical particle with temperature. In the canonical ensemble (Boltzmann distribution) it is guaranteed that the energy change per entropy change equals temperature. And the ensemble mean of the kinetic energy of a particle equals $k_B T$ in this case. Thus, if ergodicity is assumed, i.e., if the time average equals the ensemble average, temperature may indeed be defined as the time averaged kinetic energy. Similar approaches have been proposed on the basis of the microcanonical ensemble [8,9]. However, if temperature was given by a time average over an observable, the proper averaging time remains open and thus the question on what minimum timescale temperature may be defined. Furthermore, this definition was entirely based on ergodicity. Nevertheless, it allows, at least to some extent, for an investigation of processes, in which temperature varies in time and/or space, since that definition is not necessarily restricted to full equilibrium.

To avoid those problems of standard temperature definitions, we present here yet another, entirely quantum mechanical definition.

7. Definition of Spectral Temperature

We define the inverse spectral temperature as [4]

$$\frac{1}{k_B T} := - \left(1 - \frac{W_0 + W_M}{2} \right)^{-1} \sum_{i=1}^M \left(\frac{W_i + W_{i-1}}{2} \right) \frac{\ln(W_i/W_{i-1}) - \ln(N_i/N_{i-1})}{E_i - E_{i-1}}, \quad (26)$$

where W_i is the probability to find the quantum system at the energy E_i , M is the number of the highest energy level E_M , while the lowest one is labeled E_0 . This formula is motivated by the following idea: For a two level system it seems plausible to define temperature just from the energy probability distribution and the degrees of degeneracy as

$$\frac{W_1 N_0}{W_0 N_1} = \exp \left(- \frac{E_1 - E_0}{k_B T} \right). \quad (27)$$

The definition (26) results if one groups the energy levels of a multi-level system into neighboring pairs, to each of which a “temperature” is assigned via the above formula, weighted by the average probability for each pair to be occupied. This definition obviously depends only on the energy probability distribution and the spectrum of a system. It thus cannot change in time for an isolated system, and it is always defined, independent of whether or not the system is in an equilibrium state. Thus there should be many systems or situations with such a temperature, which do not exhibit thermodynamic properties at all. The latter will only show up in equilibrium situations or close to those.

If the spectrum of a system was very dense and if it was possible to describe the energy probability distribution, $\{W_i\}$, as well as the degrees of degeneracy, $\{N_i\}$, by smooth continuous functions $(W(E), N(E))$ with a well defined derivative, (26) could be approximated by

$$\frac{1}{k_B T} \approx - \int_0^{E_{\max}} W(E) \left(\frac{d}{dE} \ln W(E) - \frac{d}{dE} \right) \ln N(E) dE . \quad (28)$$

This can further be simplified by integrating the first term to yield

$$\frac{1}{k_B T} \approx W(0) - W(E_{\max}) + \int_0^{E_{\max}} \frac{W(E)}{N(E)} \frac{dN(E)}{dE} dE . \quad (29)$$

Since for larger systems typically neither the lowest nor the highest energy level is occupied with considerable probability (if the spectra are finite at all), it is the last term on the right hand side of (29), that basically matters. This term can be interpreted as the average over the standard, system based, rather than micro state based definition of the inverse temperature.

8. Equilibrium Properties of Model Systems

We now turn to some numerical data, based on a certain type of models. These models are still rather abstract and may thus be viewed as models for a whole class of bipartite systems. The subsystems g, c are specified by their respective spectra only, or, rather, those respective parts which play any role at all under the

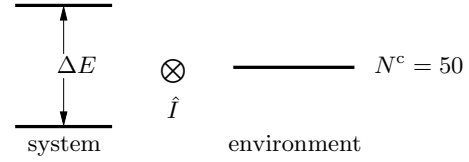


Fig. 3. Microcanonical scenario: A non-degenerate two-level-system (gas) is weakly coupled to a system with one energy level of degeneracy $N^c = 50$. This is a model for a system in contact with a much larger environment such that no energy can be exchanged between the system and environment.

condition of energy conservation. What sort of physical structure could give rise to those spectra is not considered here, since it turns out to be irrelevant to some extent.

The spectra are translated into discrete diagonal matrix Hamiltonians that describe the decoupled bipartite system. These can be chosen to be diagonal, without any loss of generality, since any such system may be analyzed in the energy eigenbasis of its decoupled parts. The form of the interaction depends on the concrete physical subsystems and their interactions. But since the “guess” is that for the quantities considered here (entropy, occupation probabilities, etc.) the concrete form of the interaction should not matter, the interaction is taken as some random matrix thus avoiding any bias. The interaction has to be “small”. In this way it is hoped that we get models that are as “typical” for general thermodynamic situations as possible. Many of the situations analyzed in this Chapter are very similar to those treated within the context of quantum master equations. But note that in order to apply the theories at hand to those systems, neither a Markovian nor a Born assumption has to hold. We simply solve the respective Schrödinger equation in finite dimensional space.

8.1. Entropy under Microcanonical Conditions

All data in our first example refer to a situation depicted in Fig. 3 (cf. [10]). The “gas” (the system under consideration) consists of a two-level system, both levels being non-degenerate ($N_0^g = N_1^g = 1$), while the “container” (the environment) consists of just one energy level with degeneracy $N^c = 50$. This is necessarily a microcanonical situation regardless of the interaction \hat{I} . The container cannot absorb any energy, therefore

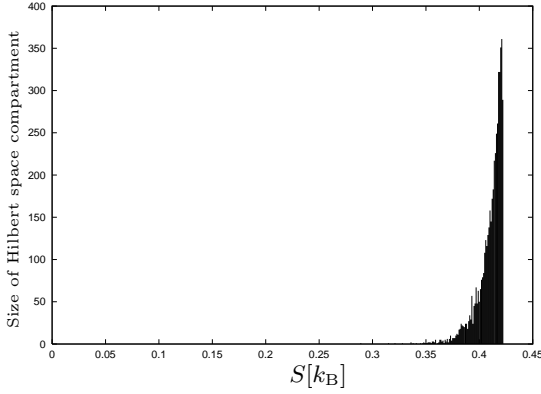


Fig. 4. Relative size of Hilbert space compartments: this histogram shows the relative frequency of states with a given local entropy S , among all states from the accessible region. In this case the maximum possible entropy is $S_{\max}^g = 0.423 k_B$. Obviously, almost all states feature entropies close to the maximum.

energy cannot be exchanged between the systems. In this situation the probabilities to find the gas system in the ground (excited) state W_0^g (W_1^g) are conserved quantities and in this example chosen as

$$W_0^g = 0.15, \quad W_1^g = 0.85. \quad (30)$$

As described in Sect. 3, the Hilbert space average of the purity of the gas system is under condition (13) given according to (14) by $\llbracket P^g \rrbracket = 0.765$. The corresponding minimum purity (9) is $P_{\min}^g = 0.745$. As explained in Sect. 3, we find here

$$\llbracket P^g \rrbracket \approx P_{\min}^g, \quad (31)$$

a situation, in which almost the entire accessible region would be filled with the compartment containing only states of almost maximum local entropy.

To confirm this expectation, a set of random states, uniformly distributed over the accessible region, has been generated. Their local entropies have been calculated and sorted into a histogram. Since those states are distributed uniformly over the accessible region, the number of states in any “entropy bin” reflects the relative size of the respective Hilbert space compartment.

The histogram is shown in Fig. 4. The maximum local entropy in this case is $S_{\max}^g = 0.423 k_B$. Obviously, almost all states have local entropies close to S_{\max}^g . Thus compartments corresponding to entropies of, say, $S^g > 0.4 k_B$ indeed fill almost the entire accessible region, just as theory predicts. Local pure states ($S^g = 0$) are practically of measure zero.

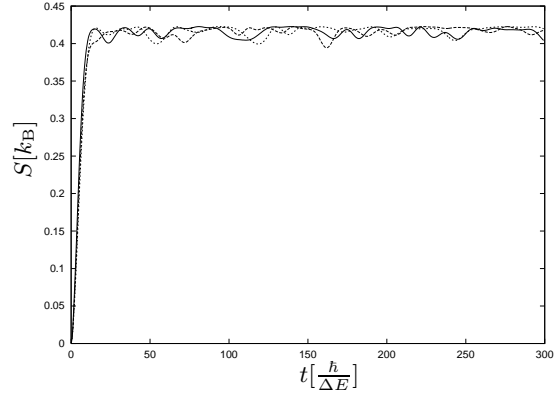


Fig. 5. Evolution of the local entropy for different initial states. A universal state of maximum entropy (equilibrium) is reached, independent of the initial state.

In order to examine the dynamics, a coupling \hat{I} is introduced. To keep the concrete example as general as possible, \hat{I} has been chosen as a random matrix in the basis of the energy eigenstates of the uncoupled system, with Gaussian distributed real and imaginary parts of the matrix elements of zero mean and a standard deviation of

$$\Delta I = 0.01 \Delta E. \quad (32)$$

This coupling is weak, compared to the Hamiltonian of the uncoupled system. Therefore the respective interaction cannot contain much energy. The spectrum of the system (see Fig. 3) does not change significantly due to the coupling, and after all the environment is not able to absorb energy.

Now the Schrödinger equation for this system, including a realization of the interaction, has been solved for initial states consistent with (30). Then the local entropy at each time has been calculated, thus getting a picture of the entropy evolution. The result is shown in Fig. 5. Obviously the entropy approaches S_{\max}^g within a reasonable time, regardless of the concrete initial state. Thus the tendency towards equilibrium is obvious. The concrete form of the interaction \hat{I} only influences the details of this evolution, the equilibrium value is always the same. If the interaction is chosen to be weaker, the time scale on which equilibrium is reached gets longer, but, eventually the same maximum entropy will be reached in any case.

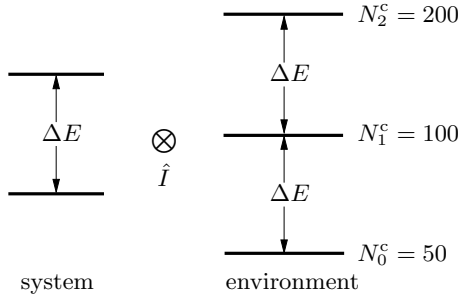


Fig. 6. Canonical scenario: A two-level gas system is weakly coupled to a three level environment, such that energy can be exchanged. The exponential degeneracy scheme of the container system guarantees a full independence of the equilibrium state from the initial state.

8.2. Occupation Probabilities under Canonical Conditions

The second model analyzed numerically is depicted in Fig. 6. The considered (gas) system, again, consists only of a non-degenerate two-level system. The environment (container) in this case is a three-level system with an exponential “state density”: $N_B^c = 50 \cdot 2^B$ with $B = 0, 1, 2$. This has been chosen since theory predicts for such a degeneracy scheme of the environment an equilibrium state of the gas system, which should be independent of its initial state (see (22)). If we restrict ourselves to initial states featuring arbitrary states for the gas system but container states that only occupy the intermediate energy level, no other container levels except for those given could be reached, even if they were present: This is due to energy conservation and holds for the limit of weak interactions \hat{I} .

In this case the model can also be seen to represent a situation with a much larger environment and we find from (23)

$$W^d(E_0^g) = \frac{2}{3}, \quad W^d(E_1^g) = \frac{1}{3}. \quad (33)$$

To keep the situation as general as possible, \hat{I} was, like in Sect. 8.1, chosen to be a matrix with random Gaussian distributed entries in the basis of the eigenstates of the uncoupled system, but now with energy transfer allowed between the subsystems.

For this system the Schrödinger equation has been solved and the evolution of the probability to find the gas system in its ground state, $W(E_0^g)$ is displayed in Fig. 7. The different curves correspond to different interaction strengths, given by the standard deviation

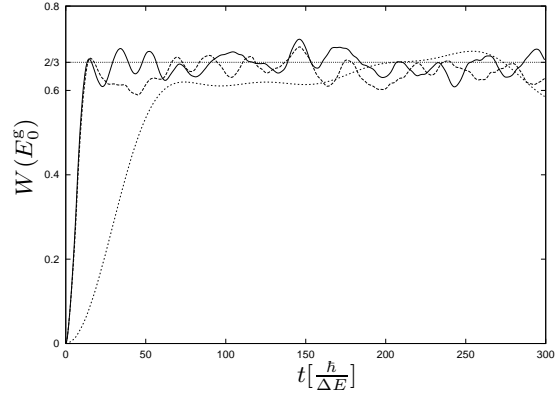


Fig. 7. Evolution of the ground level occupation probability for three different random interactions. The dotted line corresponds to a weaker interaction. Even in this case the same equilibrium value, $W_A^d = \frac{2}{3}$, is approached, only on a longer timescale.

of the distribution of the matrix elements of \hat{I} , ΔI :

$$\Delta I_{\text{solid, dashed}} = 0.0075\Delta E, \quad \Delta I_{\text{dotted}} = 0.002\Delta E. \quad (34)$$

Obviously, the equilibrium value of $W^d(E_0^g) = 2/3$ is reached independently of the concrete interaction \hat{I} . Within the weak coupling limit the interaction strength only influences the timescale on which equilibrium is reached.

Figure 8 displays the evolution of the same probability, $W(E_0^g)$, but now for different initial states, featuring different probabilities for the groundstate, as can be seen in the figure at $t = 0$. The equilibrium value is reached for any such evolution, regardless of the special initial state, thus we confirm the effective attractor behavior typical for thermodynamics.

Figure 9 shows the evolution of the local entropy of the gas system for the same three initial states as used for Fig. 8.

The maximum entropy, consistent with the equilibrium value of the energy probabilities, is $S_{\text{max}}^g = 0.637 k_B$. This is also the value one finds, if one maximizes entropy for fixed mean energy (Jaynes’ principle [11]). Obviously, this value is reached for any initial state during the concrete dynamics of this model. This supports the validity of (20), which states that the density matrix of the equilibrium state is diagonal in the basis of the local energy eigenstates.

To analyze the formation of a full Boltzmann distribution, we turn to the system depicted in Fig. 10. Here the “gas” system is a non-degenerate equidistant five-

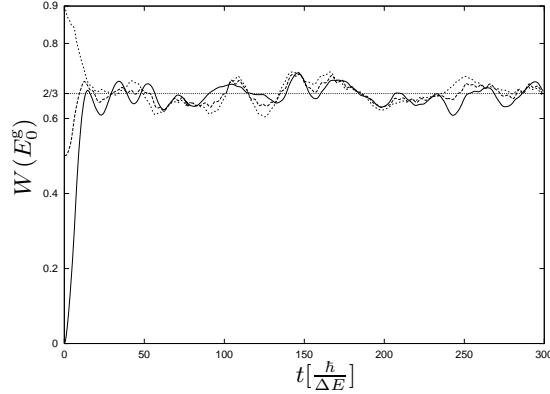


Fig. 8. Evolution of the ground level occupation probability for different initial states. The theoretically predicted equilibrium value is reached, independent of the initial states, as expected for canonical conditions.

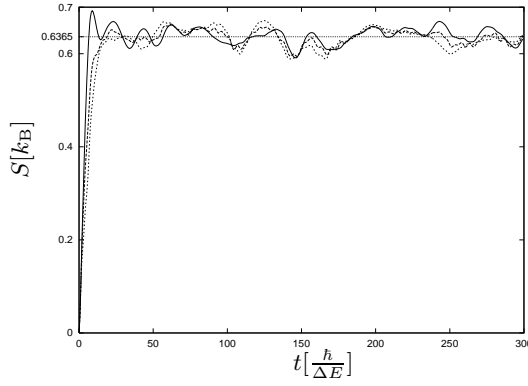


Fig. 9. Evolution of the local entropy for different initial states. $S = 0.637 k_B$ is the maximum entropy that is consistent with the equilibrium energy probabilities. This maximum entropy state is reached in all cases.

level system the container system a five-level system with degeneracies $N_B^c = 6 \cdot 2^B$ ($B = 0, \dots, 4$), which should lead to a Boltzmann distribution. We restrict ourselves to initial states, where for both subsystems only the intermediate energy level is occupied (symbolized by the black dots in Fig. 10). Due to energy conservation other states of the container system would not play any role in this case even if they were present, just like in the previous model. Figure 11 shows the probabilities of the different energy levels to be occupied $W(E_A^g)$. While the gas system starts in the intermediate (third) energy level, soon a Boltzmann distribution develops: Obviously, each probability becomes twice as high as the one for the level above. This is exactly what theory predicts (see (18)) for the environ-

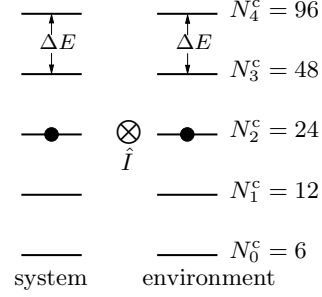


Fig. 10. Canonical multi-level scenario: A five-level gas system is weakly coupled to a five level container system with an exponential degeneracy scheme, such that energy may be exchanged. Black dots symbolize the initial state. This set-up should lead to a Boltzmann distribution.

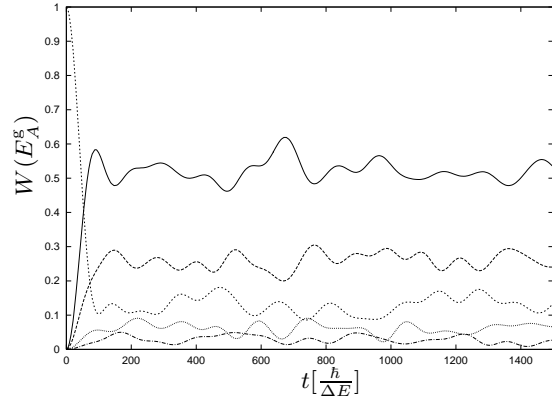


Fig. 11. Evolution of the energy occupation probabilities. After some relaxation time a Boltzmann distribution is reached. Each probability is twice as high as the one for the next higher energy level, as theory predicts.

ment degeneracy scheme under consideration.

8.3. Probability Fluctuations

Finally, we consider fluctuations in time due to finite size effects imposed by the environment. For this purpose a system almost like the one depicted in Fig. 6 is analyzed, but now with a degeneracy scheme given by

$$N_B^c = \frac{N_1^c}{2} \cdot 2^B. \quad (35)$$

The ratios between the degrees of degeneracy of the different container levels are thus the same as for the system sketched in Fig. 6, but the overall size of the container system is tunable by N_1^c . For various N_1^c , the Schrödinger equation has been solved numerically,

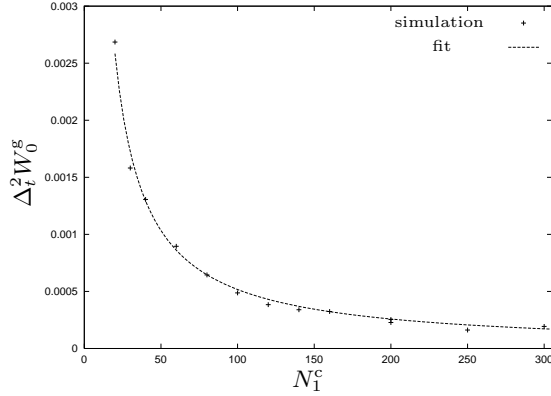


Fig. 12. Fluctuations of the probability for the considered system to be in the ground state $\Delta_t W_0^g$, in dependence on the number of eigenstates of the environment system N_1^c . Obviously, the fluctuations go down, with increasing environment.

and the following measure of the fluctuations of the occupation probability of the ground level of the gas system has been computed

$$\Delta_t^2 W_0^g := \frac{1}{t_f - t_i} \left(\int_{t_i}^{t_f} (W_0^g(t))^2 dt - \left(\int_{t_i}^{t_f} W_0^g(t) dt \right)^2 \right), \quad (36)$$

for initial states with

$$W_0^g(0) = 0.2, \quad W_1^g(0) = 0.8. \quad (37)$$

Figure 12 shows the dependence of the size of these fluctuations on the container system size N_1^c . The small crosses are the computed data points, the dashed line is a least square fit to a function proportional to $1/N_1^c$,

$$\Delta_t W_0^g = \sqrt{\frac{0.053}{N_1^c}}. \quad (38)$$

This fit is in very good agreement with the theoretical expectation, although the trajectories are not ergodic.

9. Summary and Conclusions

The reduction of thermodynamics to an underlying theory has challenged physicists for more than a century. So far such attempts have met with partial success only. In this context an interesting and, as we believe, consistent route is offered by quantum thermodynamics.

Quantum thermodynamics as a concept has not yet a generally accepted meaning (see, e.g. [12] for a different opinion). Our version has been introduced as a special field within decoherence theory. It makes use of a special methodology, which is based on statistical techniques to investigate the structure of a product Hilbert space under certain constraints. These constraints, though, are by themselves emergent properties of the system environment model.

Within this quantum thermodynamics we are able to show that thermodynamics is already contained in the deterministic Schrödinger dynamics. Fingerprints of equilibrium behavior show up already in surprisingly small bipartite quantum systems. As a consequence thermodynamics need not be considered as a final remedy after all detailed microscopic descriptions have failed: Deterministic Schrödinger dynamics of the whole and (apparent) relaxation behavior of the embedded part is no contradiction at all.

Such a picture should also give new insight on thermodynamic applications in the nano-regime [13]. This expectation is corroborated by the fact that pertinent models then have to be on the quantum level anyway, while the conditions for a thermodynamic description can be made explicit, as this is part of the complete quantum description of system and environment [14].

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